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Fleming's bound for the decay of mixed states

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Abstract. Fleming's inequality is generalized to the decay function of mixed states. We show that for any symmetric hamiltonian h and for any density operator ρ on a finite dimensional Hilbert space with the orthogonal projection Π onto the range of ρ there holds the estimate $\mathrm{Tr}(\Pi e^{-iht}\rho e^{iht}) \geq \cos^2((\Delta h)_\rho t)$ for all real t with $(\Delta h)_\rho |t| \leq \pi/2$. We show that equality either holds for all $t \in \mathbb{R}$ or it does not hold for a single t with $0 < (\Delta h)_\rho |t| \leq \pi/2$. All the density operators saturating the bound for all $t \in \mathbb{R}$, i.e. the mixed intelligent states, are determined.

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1. Introduction

Two states ρ_1 and ρ_2 of a quantum system can be discriminated on the basis of a single measurement outcome if there exists an observable A such that the probability measures which are generated by ρ_1 and ρ_2 on the spectrum of A have disjoint supports. In particular if a state ρ evolves under a Hamiltonian H into the state ρ_t it may be desirable to determine and perhaps to minimize a time $t > 0$ when the evolved state ρ_t can be discriminated from the initial state ρ by a single measurement. A more realistic goal is to distinguish ρ_t from ρ by performing single measurements on "few" ensemble members only. If one chooses as observable A an orthogonal projection Π with $\mathrm{Tr}\,(\Pi\rho) = 1$, then this can be done if $\mathrm{Tr}\,(\Pi\rho_t)$ is close to 0 since this means that it is very unlikely to find the property Π in the state ρ_t, while it is certain in the state ρ.

Under a somewhat broader perspective the quantity $\mathrm{Tr}\,(\Pi\rho_t)$ is commonly used in order to formalize the intuitive picture of the decay of a property. [1] Since in many cases the survival probability $\mathrm{Tr}\,(\Pi\rho_t)$ of the property Π cannot be computed explicitly, there arises the quest for estimates of the decay-function $P_\rho : t \mapsto \mathrm{Tr}\,(\Pi\rho_t)$.

An important such estimate for P_ρ in the case of a pure state ρ and in case of the property $\Pi = \rho$ is due to Mandelstam and Tamm [2]. This estimate has been rediscovered by a different reasoning almost 30 years later by Fleming. [3] Since then it is called Fleming's bound. It says that for any pure state ρ with a finite energy uncertainty $(\Delta H)_\rho$ there holds

$$P_\rho\,(t) \geq \cos^2 \frac{(\Delta H)_\rho\, t}{\hbar} \text{ for all } t \text{ with } \frac{(\Delta H)_\rho\,|t|}{\hbar} \leq \pi/2. \tag{1}$$

From the estimate (1) a lower bound to any positive t such that $\mathrm{Tr}\,(\Pi\rho_t) = \varepsilon$ is obvious‡:

$$\frac{\hbar}{(\Delta H)_\rho} \arccos \sqrt{\varepsilon} \leq t.$$

The special case $\varepsilon = 0$ leads to the inequality

$$\frac{\pi\hbar}{2\,(\Delta H)_\rho} \leq t \tag{2}$$

for the smallest time $t > 0$ with $\mathrm{Tr}\,(\Pi\rho_t) = 0$. This time, if existent, is called orthogonalization [4] or passage time [5]. Clearly it would also be useful to have an upper bound for P_ρ, from which the existence of an orthogonalization time could be inferred. Polynomial upper bounds have been given by Andrews [6], which, however, are strictly positive. Therefore they do not yield an upper bound to an orthogonalization time.

A simple geometric meaning of Fleming's bound became clear through the time-energy uncertainty relation of Aharonov and Anandan [7]: First, $2t\,(\Delta H)_\rho/\hbar$ equals the arc length of the curve $\lambda \mapsto \rho_\lambda$ with $0 \leq \lambda \leq t$ in the projective space $\mathcal{P}(\mathcal{H})$ of one dimensional subspaces of $\mathcal{H}$. Second, $2 \arccos \sqrt{P_\rho(t)}$ equals the geodesic distance between ρ and ρ_t in $\mathcal{P}(\mathcal{H})$. Here the Riemannian geometry is defined by the Fubini-Study metric of $\mathcal{P}(\mathcal{H})$. Thus, as has been pointed out by Brody [5], Fleming's bound (1) is equivalent to the fact that the length of a curve in $\mathcal{P}(\mathcal{H})$ is not less than the geodesic distance between its initial and end point.

In Ref. [8] for given Hamiltonian H all pure states ρ with an orthogonalization time equal to the lower bound $\pi\hbar/2\,(\Delta H)_\rho$ of equation (2) have been identified. I.e., for such states there holds $(\Delta H)_\rho\, t = \hbar\pi/2$ for the smallest $t > 0$ with $P_\rho(t) = 0$. These states are called "intelligent states" as they saturate the Aharonov-Anandan uncertainty relation. A pure state ρ is found to be intelligent if and only if there exist two eigenvectors ϕ_1, ϕ_2 of H corresponding to different eigenvalues and with $\|\phi_1\| = \|\phi_2\|$ such that ρ equals the orthogonal projection onto the one dimensional subspace $\mathbb{C} \cdot (\phi_1 + \phi_2)$. [8]

In [5] a lower bound for the smallest $t > 0$ with $P_\rho(t) = 0$ is given for a special type of a mixed states: The density operator ρ is assumed to be a mixture of mutually orthogonal intelligent pure states. In Ref. [4] a generalization of the orthogonalization time to mixed states has been addressed too. In this work, however, the fidelity $\mathrm{Tr}\,\sqrt{\sqrt{\rho}\rho_t\sqrt{\rho}}$ is used as a measure of the degree of decay. Clearly, for mixed states the fidelity does not coincide with $\mathrm{Tr}\,(\Pi\rho_t)$. So neither of the two works [5], and [4] presents a generalization of Fleming's bound (1) to the case of an arbitrary mixed state.

In this paper we generalize Fleming's bound to an arbitrary mixed state ρ. We consider the decay function $P_\rho(t) = \mathrm{Tr}\,(\Pi\rho_t)$, where Π is chosen to be the orthogonal projection onto the range of ρ and we confine ourselves to finite dimensional Hilbert spaces. We first extend Fleming's bound to P_ρ. We then sharpen the bound by proving that only one of the two cases

(i) $P_\rho(t) > \cos^2\left((\Delta H)_\rho\, t/\hbar\right)$ for all t with $0 < (\Delta H)_\rho\, |t|/\hbar \leq \pi/2$

‡ Clearly this does not imply that there exists any t at all such that $P_\rho(t) = \varepsilon$ holds.

(ii) $P_\rho(t) = \cos^2\left((\Delta H)_\rho\, t/\hbar\right)$ for all $t \in \mathbb{R}$

is realized. Then we identify the set of all density operators which saturate Fleming's bound. In order to have the paper reasonably selfcontained we have included a treatment of some closely related well known results on pure state decay. In this way it also becomes more visible which structures remain unchanged when going from pure states to mixed ones. The pure state decay function P_ρ is denoted as P_ϕ when $\rho = \phi\langle\phi,\cdot\rangle$.

2. Pure state decay

Let $\mathcal{H}$ be a finite dimensional Hilbert space. The scalar product of two vectors $\phi, \psi \in \mathcal{H}$ is denoted by $\langle\phi,\psi\rangle$. Let the dynamics of $\mathcal{H}$ be given in terms of a symmetric linear operator $h : \mathcal{H} \to \mathcal{H}$ by $\phi_t = \exp(-\mathrm{i}ht)\,\phi$ for $t \in \mathbb{R}$ and $\phi \in \mathcal{H}$. The survival amplitude $A_\phi : \mathbb{R} \to \mathbb{C}$ is defined for $\phi \in \mathcal{H}$ with $\|\phi\| = 1$ through $A_\phi(t) = \langle\phi,\phi_t\rangle$ and accordingly the survival probability of ϕ as a function of t is given by $P_\phi = |A_\phi|^2 : \mathbb{R} \to \mathbb{R}_{\geq 0}$. From the Cauchy-Schwarz inequality we have $P_\phi \leq 1$. The nonnegative number $P_\phi(t)$ is the probability that the pure state $\phi_t\langle\phi_t,\cdot\rangle$ passes a preparatory filter for the state $\phi\langle\phi,\cdot\rangle$. Due to

$$A_\phi(-t) = \overline{A_\phi(t)}$$

P_ϕ is an even function. Since $\phi_0 = \phi$ we have $A_\phi(0) = 1 = P_\phi(0)$.

The expectation value of h in the state $\phi\langle\phi,\cdot\rangle$ is denoted by $\langle h\rangle_\phi = \langle\phi, h\phi\rangle$ and its variance reads

$$(\Delta h)^2_\phi = \left\langle h^2\right\rangle_\phi - \langle h\rangle^2_\phi .$$

ϕ is an eigenvector of h if and only if $(\Delta h)_\phi = 0$. Thus for $(\Delta h)_\phi = 0$ the function P_ϕ is constant, i.e. $P_\phi(t) = 1$ holds for all t. For $(\Delta h)_\phi > 0$, however, P_ϕ is not constant since for $t \to 0$

$$\begin{aligned} P_\phi(t) &= \left|1 - \mathrm{i}t\langle h\rangle_\phi - \frac{1}{2}t^2\left\langle h^2\right\rangle_\phi + \mathrm{i}\frac{1}{3!}t^3\left\langle h^3\right\rangle_\phi + \mathrm{O}\left(t^4\right)\right|^2 \\ &= \left(1 - \frac{1}{2}t^2\left\langle h^2\right\rangle_\phi\right)^2 + \left(t\langle h\rangle_\phi - \frac{1}{3!}t^3\left\langle h^3\right\rangle_\phi\right)^2 + \mathrm{O}\left(t^4\right) \\ &= 1 - (\Delta h)^2_\phi\, t^2 + \mathrm{O}\left(t^4\right). \end{aligned}$$

Thus P_ϕ has a strict local maximum at $t = 0$ if and only if $(\Delta h)_\phi > 0$.

Due to the spectral theorem there exist (unique) nonzero pairwise orthogonal vectors $\phi_1, \ldots \phi_n$ with $h\phi_\alpha = \omega_\alpha\phi_\alpha$ and $\omega_1 < \ldots < \omega_n$ such that

$$\phi_t = \mathrm{e}^{-\mathrm{i}\omega_1 t}\phi_1 + \ldots + \mathrm{e}^{-\mathrm{i}\omega_n t}\phi_n$$

for all t. Then $A_\phi(t) = \sum_{\alpha=1}^n \lambda_\alpha \mathrm{e}^{-\mathrm{i}\omega_\alpha t}$ with $\lambda_\alpha = \|\phi_\alpha\|^2 > 0$ follows. For $P_\phi(t)$ one obtains

$$P_\phi(t) = \sum_{\alpha,\beta=1}^n \lambda_\alpha\lambda_\beta \mathrm{e}^{-\mathrm{i}(\omega_\alpha-\omega_\beta)t} = \sum_{\alpha,\beta=1}^n \lambda_\alpha\lambda_\beta \cos\left[(\omega_\alpha - \omega_\beta)\,t\right]. \qquad (3)$$

Thus both A_ϕ and P_ϕ are the restriction of an entire function to the real line. In particular A_ϕ and P_ϕ are C^∞ functions.

It has been shown by Mandelstam and Tamm [2], and along a different strategy by Fleming in [3] that for all t with $(\Delta h)_\phi |t| \leq \pi/2$ there holds

$$P_\phi(t) \geq \cos^2\left((\Delta h)_\phi t\right).$$

The original proof of Mandelstam and Tamm [2] has been elaborated by Schulmann in [9]. A new proof has been given recently by Kosiński and Zych. [10]

We shall now prove the following somewhat stronger result implicitly contained in [4] and [5].

Proposition 1 *Let $\phi \in \mathcal{H}$ with $\|\phi\| = 1$ and $(\Delta h)_\phi > 0$. Then exactly one of the alternatives (i) and (ii) holds.*

(i) $P_\phi(t) > \cos^2\left((\Delta h)_\phi t\right)$ *for all* $t \in \mathbb{R}$ *with* $0 < (\Delta h)_\phi |t| \leq \pi/2$

(ii) $P_\phi(t) = \cos^2\left((\Delta h)_\phi t\right)$ *for all* $t \in \mathbb{R}$

Alternative (ii) holds if and only if there exist two vectors $\phi_1, \phi_2 \in \mathcal{H}$ with $h\phi_i = \omega_i \phi_i,\ \omega_1 < \omega_2,\ \|\phi_i\|^2 = 1/2$ such that $\phi = \phi_1 + \phi_2$.

Proof. Let $\Pi = \phi \langle \phi, \cdot \rangle$. Then holds $P_\phi(t) = \left\langle \phi, \mathrm{e}^{\mathrm{i}ht} \Pi \mathrm{e}^{-\mathrm{i}ht} \phi \right\rangle = \langle \Pi \rangle_{\phi_t}$. From this it follows that

$$\frac{\mathrm{d}}{\mathrm{d}t} P_\phi(t) = \mathrm{i} \left\langle \phi, \mathrm{e}^{\mathrm{i}ht} [h, \Pi] \mathrm{e}^{-\mathrm{i}ht} \phi \right\rangle = \mathrm{i} \langle [h, \Pi] \rangle_{\phi_t}.$$

Using the uncertainty relation for the pair (h, Π) we thus obtain for $P'_\phi(t) = \frac{\mathrm{d}}{\mathrm{d}t} P_\phi(t)$ the estimate

$$\left|P'_\phi(t)\right| = \left|\langle [h, \Pi] \rangle_{\phi_t}\right| \leq 2 (\Delta h)_\phi (\Delta \Pi)_{\phi_t}.$$

From $(\Delta\Pi)^2_{\phi_t} = \left\langle \Pi^2 \right\rangle_{\phi_t} - \langle \Pi \rangle^2_{\phi_t} = \langle \Pi \rangle_{\phi_t} - \langle \Pi \rangle^2_{\phi_t} = \langle \Pi \rangle_{\phi_t} \left(1 - \langle \Pi \rangle_{\phi_t}\right)$ it follows that for all $t \in \mathbb{R}$

$$\left|P'_\phi(t)\right| \leq 2 (\Delta h)_\phi \sqrt{P_\phi(t) \left(1 - P_\phi(t)\right)}. \tag{4}$$

We first simplify this inequality by introducing the dimensionless time variable $x = t (\Delta h)_\phi$ and the function $v : \mathbb{R} \to [0,1]$ with $v(x) = P_\phi(t)$. Inequality (4) then becomes equivalent to

$$-2\sqrt{v(x)(1 - v(x))} \leq v'(x) \leq 2\sqrt{v(x)(1 - v(x))} \text{ for all } x \in \mathbb{R}.$$

In order to make use of the differential inequality

$$-2\sqrt{v(x)(1 - v(x))} \leq v'(x) \tag{5}$$

we first discuss the (autonomous) differential equation

$$y' = f(x, y) \ \text{ with } f : \mathbb{R} \times (0,1) \to \mathbb{R},\ f(x,y) = -2\sqrt{y(1-y)}. \tag{6}$$

The function $y_0 : (0, \pi/2) \to (0,1)$ with $y_0(x) = \cos^2 x$ is a solution of this differential equation since for all $x \in (0, \pi/2)$

$$y_0'(x) = -2\cos(x)\sin(x) = -2\sqrt{y_0(x)}\sqrt{1 - y_0(x)} = f(x, y_0(x)).$$

This solution of (6) is of maximal domain since the limits

$$\lim_{x\to 0} y_0\,(x) = 1 \text{ and } \lim_{x\to \pi/2} y_0\,(x) = 0$$

do not belong the admitted range $0 < y < 1$ of solutions. Other solutions of maximal domain are obtained from y_0 by translation: $y_c\,(x) = y_0\,(x-c)$ for $c < x < c+\pi/2$. By a suitable choice of c the initial value problem $y_c\,(\xi) = \eta$ for any $(\xi,\eta) \in \mathbb{R}\times(0,1)$ is solved. Since f obeys the local Lipschitz condition of the uniqueness theorem for the solutions of first order differential equations, the set of all solutions to $y' = f\,(x,y)$ with maximal domain is given by $\{y_c\,|c \in \mathbb{R}\}$.

The continuous extension g of f to the domain $\mathbb{R}\times[0,1]$ leads to the differential equation $z' = g\,(x,z) = -2\sqrt{z\,(1-z)}$ which violates the local Lipschitz condition on the boundary points (x,z) with either $z=0$ or $z=1$. The set of solutions of the extended equation with maximal domain is given by $\{z_c\,|c\in\mathbb{R}\}$ with

$$z_c : \mathbb{R}\to\mathbb{R},\; z_c\,(x) = \begin{cases} 1 & \text{for } x < c \\ \cos^2(x-c) & \text{for } c \le x \le c+\pi/2 \\ 0 & \text{for } x > c+\pi/2 \end{cases}$$

Thus any function z_c with $c \ge 0$ is a solution of the initial value problem $z\,(0) = 1$ with maximal domain. For any such solution z_c with $c \ge 0$ holds

$$z_0\,(x) \le z_c\,(x) \le 1$$

for all $x \ge 0$.

According to a theorem of differential inequalities, quoted in the appendix A, we then conclude from (5) and from $v\,(0) = 1$ that for all $x \ge 0$

$$v\,(x) \ge z_0\,(x)\,.$$

Thus $v\,(x) \ge \cos^2 x$ for all $x \in [0,\pi/2]$. This is Fleming's inequality.

Suppose now that $\eta := v(\xi) > \cos^2\xi$ for some $\xi \in (0,\pi/2)$. With $\eta = \cos^2(\xi - c)$ for some $c \in (0,\pi/2)$ it then follows again from the quoted theorem on differential inequalities that $v\,(x) \ge \cos^2(x-c) > \cos^2(x)$ for all $x \in [\xi,\pi/2]$. From Fleming's inequality we now have the two cases only:

(i) For any $\varepsilon > 0$ there exists a $\xi \in (0,\varepsilon)$ with $v(\xi) > \cos^2\xi$.

(ii) There exists an $\varepsilon > 0$ with $v\,(x) = \cos^2 x$ for all $x \in (0,\varepsilon)$.

In the case (i) we have $v\,(x) \ge \cos^2(x-c) > \cos^2(x)$ for all $x \in [\xi,\pi/2]$. Since there exist such ξ arbitrarily close to 0 it follows that $v\,(x) > \cos^2(x)$ for all $x \in (0,\pi/2]$. Since v is an even function the inequality extends to all x with $|x| \in (0,\pi/2]$.

In case of (ii) the identity theorem of holomorphic functions implies $v\,(x) = \cos^2(x)$ for all $x \in \mathbb{R}$ since v is the restriction of an entire function to the real line. Thus we have derived the alternatives (i) and (ii) as being exhaustive.

Suppose now that alternative (ii) holds. From the spectral decomposition (3) of P_ϕ we extract the constant term and the one with the highest frequency according to

$$\begin{aligned} P_\phi(t) &= \sum_{\alpha=1}^{n} \lambda_\alpha^2 + 2 \sum_{\substack{\alpha,\beta=1 \\ \alpha>\beta}}^{n} \lambda_\alpha \lambda_\beta \cos\left[(\omega_\alpha - \omega_\beta) t\right] \\ &= \sum_{\alpha=1}^{n} \lambda_\alpha^2 + 2\lambda_n \lambda_1 \cos\left[(\omega_n - \omega_1) t\right] + 2 \sum_{\substack{\alpha,\beta=1 \\ \alpha>\beta, (\alpha,\beta)\neq(n,1)}}^{n} \lambda_\alpha \lambda_\beta \cos\left[(\omega_\alpha - \omega_\beta) t\right]. \end{aligned}$$

The assumption $P_\phi(t) = \cos^2\left((\Delta h)_\phi t\right) = \frac{1}{2}\left(1 + \cos\left(2(\Delta h)_\phi t\right)\right)$ now implies, due to $\lambda_\alpha \lambda_\beta > 0$ for all α, β, that the index set of the last sum is empty. Thus we have $n = 2$ and

$$\lambda_1^2 + \lambda_2^2 = \frac{1}{2},\ 2\lambda_1\lambda_2 = \frac{1}{2},\ \omega_2 - \omega_1 = 2(\Delta h)_\phi .$$

The first two equations imply $\lambda_1 = \lambda_2 = 1/2$. From this it follows that the third condition $\omega_2 - \omega_1 = 2(\Delta h)_\phi$ holds, since

$$\begin{aligned} (\Delta h)_\phi^2 &= \lambda_1 \omega_1^2 + \lambda_2 \omega_2^2 - (\lambda_1\omega_1 + \lambda_2\omega_2)^2 \\ &= \frac{1}{2}\left(\omega_1^2 + \omega_2^2\right) - \frac{1}{4}(\omega_1 + \omega_2)^2 \\ &= \frac{1}{4}(\omega_1 - \omega_2)^2 . \end{aligned}$$

Thus we have derived from alternative (ii) that ϕ is a linear combination of just two eigenvectors of h with spectral components of equal norm. The inverse conclusion that alternative (ii) follows from $\phi = \phi_1 + \phi_2$ with $h\phi_i = \omega_i \phi_i, \omega_2 > \omega_1$ and $\|\phi_i\|^2 = \lambda_i = 1/2$ is obvious from

$$\begin{aligned} P_\phi(t) &= \lambda_1^2 + \lambda_2^2 + 2\lambda_1\lambda_2 \cos\left[(\omega_2 - \omega_1) t\right] \\ &= \frac{1}{2}\left(1 + \cos\left[(\omega_2 - \omega_1) t\right]\right) = \cos^2\left((\Delta h)_\phi t\right). \end{aligned}$$

■

3. Mixed state decay

Let $\rho : \mathcal{H} \to \mathcal{H}$ be a density operator on the finite dimensional Hilbert space $\mathcal{H}$, i.e. ρ is linear with $\rho \geq 0$ and $\mathrm{Tr}(\rho) = 1$. Due to the spectral theorem there exist mutually orthogonal vectors $\psi_1, \ldots \psi_n$ with $\|\psi_k\| = 1$ for all k and there exist numbers $\lambda_1, \ldots \lambda_n \in \mathbb{R}_{>0}$ with $\sum_{k=1}^{n} \lambda_k = 1$ such that

$$\rho = \sum_{k=1}^{n} \lambda_k \psi_k \langle \psi_k, \cdot \rangle . \tag{7}$$

The orthogonal projection $\Pi : \mathcal{H} \to \mathcal{H}$ onto the range of ρ is given by

$$\Pi = \sum_{k=1}^{n} \psi_k \langle \psi_k, \cdot \rangle .$$

The projection Π is the smallest orthogonal projection with $\mathrm{Tr}(\rho\Pi) = 1$.

For an arbitrary orthogonal projection $E : \mathcal{H} \to \mathcal{H}$ the nonnegative number $\mathrm{Tr}\,(\rho E)$ is the probability that the state ρ passes a filter for the property associated with E. More generally, the expectation value of a linear symmetric operator $A : \mathcal{H} \to \mathcal{H}$ is given by $\langle A \rangle_\rho = \mathrm{Tr}\,(A\rho)$ and its variance reads $(\Delta A)_\rho^2 = \left\langle A^2 \right\rangle_\rho - \langle A \rangle_\rho^2$.

The dynamics $\phi \mapsto \phi_t = \exp(-\mathrm{i}ht)\,\phi$ is extended from vectors to density operators through $\rho \mapsto \rho_t = \mathrm{e}^{-\mathrm{i}ht}\rho\mathrm{e}^{\mathrm{i}ht}$. As a generalization of the survival probability to mixed states one may consider the function $P_\rho : \mathbb{R} \to [0,1]$ with

$$P_\rho\,(t) = \mathrm{Tr}\left(\Pi \mathrm{e}^{-\mathrm{i}ht}\rho\mathrm{e}^{\mathrm{i}ht}\right) = \left\langle \mathrm{e}^{\mathrm{i}ht}\Pi\mathrm{e}^{-\mathrm{i}ht}\right\rangle_\rho = \langle \Pi \rangle_{\rho_t}\,.$$

The number $P_\rho\,(t)$ thus gives the probability that the evolved state ρ_t has the property Π associated with the initial state ρ. Again $t = 0$ is an absolute maximum of P_ρ since $P_\rho\,(0) = 1$. From this it follows that $P'_\rho\,(0) = 0$ since P_ρ is differentiable.

Let $\Phi_1, \ldots \Phi_q$ with $q \geq n$ be an orthonormal basis of $\mathcal{H}$ such that $h\Phi_r = \omega_r\Phi_r$ for $r = 1, \ldots q$. Then holds

$$\begin{aligned} P_\rho\,(t) &= \mathrm{Tr}\left(\mathrm{e}^{\mathrm{i}ht}\Pi\mathrm{e}^{-\mathrm{i}ht}\rho\right) = \sum_{r=1}^{q} \left\langle \Phi_r, \mathrm{e}^{\mathrm{i}ht}\Pi\mathrm{e}^{-\mathrm{i}ht}\rho\Phi_r \right\rangle \\ &= \sum_{r,s=1}^{q} \mathrm{e}^{\mathrm{i}(\omega_r-\omega_s)t} \left\langle \Phi_r, \Pi\Phi_s \right\rangle \left\langle \Phi_s, \rho\Phi_r \right\rangle\,. \end{aligned}$$

Thus P_ρ is a finite linear combination of exponentials and thus of C^∞ type.

As in the case of pure states the condition $(\Delta h)_\rho = 0$ implies $P_\rho\,(t) = 1$ for all t. This can be seen as follows

$$\begin{aligned} 0 = (\Delta h)_\rho^2 &= \left\langle h^2 \right\rangle_\rho - \langle h \rangle_\rho^2 = \left\langle \left(h - \langle h \rangle_\rho\right)^2 \right\rangle_\rho \\ &= \sum_{k=1}^{n} \lambda_k \left\| \left(h - \langle h \rangle_\rho\right)\psi_k \right\|^2. \end{aligned}$$

Thus we have $(h - \langle h \rangle_\rho)\psi_k = 0$ for all k. Therefore all the vectors ψ_k contributing to the spectral decomposition of ρ are eigenvectors of h (with the same eigenvalue). From this then follows the stationarity of ρ, i.e. $\rho_t = \rho$ for all t. While in the case of pure states the condition $(\Delta h)_\phi > 0$ implies that P_ϕ is not constant, this is not so with mixed states. A counterexample is provided by any ρ such that Π commutes with h as it is, e.g., the case for $\rho\,(\mathcal{H}) = \mathcal{H}$, since then $\Pi = id_{\mathcal{H}}$.

In order to better understand P_ρ near 0 we first observe

$$\begin{aligned} P_\rho\,(t) &= \mathrm{Tr}\left(\Pi\mathrm{e}^{-\mathrm{i}ht}\rho\mathrm{e}^{\mathrm{i}ht}\right) = \sum_{k=1}^{n} \left\langle \psi_k, \mathrm{e}^{-\mathrm{i}ht}\rho\mathrm{e}^{\mathrm{i}ht}\psi_k \right\rangle \\ &= \sum_{k,l=1}^{n} \left\langle \psi_k, \mathrm{e}^{-\mathrm{i}ht}\psi_l \right\rangle \lambda_l \left\langle \psi_l, \mathrm{e}^{\mathrm{i}ht}\psi_k \right\rangle = \sum_{k,l=1}^{n} \lambda_l \left|\left\langle \psi_k, \mathrm{e}^{-\mathrm{i}ht}\psi_l \right\rangle\right|^2 \\ &= \sum_{k=1}^{n} \lambda_k \left|\left\langle \psi_k, \mathrm{e}^{-\mathrm{i}ht}\psi_k \right\rangle\right|^2 + \sum_{\substack{k,l=1 \\ k\neq l}}^{n} \lambda_l \left|\left\langle \psi_k, \mathrm{e}^{-\mathrm{i}ht}\psi_l \right\rangle\right|^2. \end{aligned}$$

We thus have

$$P_\rho(t) = \sum_{k=1}^{n} \lambda_k P_{\psi_k}(t) + \sum_{\substack{k,l=1 \\ k \neq l}}^{n} \lambda_l \left|\left\langle \psi_k, \mathrm{e}^{-\mathrm{i}ht} \psi_l \right\rangle\right|^2 . \tag{8}$$

The Taylor expansion of P_ρ at 0 now yields

$$\begin{aligned} P_\rho(t) &= \sum_{k=1}^{n} \lambda_k \left(1 - (\Delta h)^2_{\psi_k} t^2\right) + t^2 \sum_{\substack{k,l=1 \\ k \neq l}}^{n} \lambda_l \left|\langle \psi_k, h\psi_l \rangle\right|^2 + \mathrm{O}\left(t^3\right) \\ &= 1 - t^2 \sum_{k=1}^{n} \lambda_k (\Delta h)^2_{\psi_k} + t^2 \sum_{\substack{k,l=1 \\ k \neq l}}^{n} \lambda_l \left|\langle \psi_k, h\psi_l \rangle\right|^2 + \mathrm{O}\left(t^3\right) . \end{aligned}$$

From this we infer

$$-\frac{P''_\rho(0)}{2} = \sum_{k=1}^{n} \lambda_k (\Delta h)^2_{\psi_k} - \sum_{\substack{k,l=1 \\ k \neq l}}^{n} \lambda_l \left|\langle \psi_k, h\psi_l \rangle\right|^2 . \tag{9}$$

We shall now prove a generalization of Fleming's bound to the survival probability of mixed states.

Proposition 2 *Let $\rho : \mathcal{H} \to \mathcal{H}$ be a density operator such that $(\Delta h)_\rho > 0$. Then exactly one of the alternatives (i) and (ii) holds.*

(i) $P_\rho(t) > \cos^2\left((\Delta h)_\rho t\right)$ *for all* $t \in \mathbb{R}$ *with* $0 < (\Delta h)_\rho |t| \leq \pi/2$

(ii) $P_\rho(t) = \cos^2\left((\Delta h)_\rho t\right)$ *for all* $t \in \mathbb{R}$

Alternative (ii) holds if and only if there exist two (different) eigenvalues ω_1, ω_2 of h such that every vector ψ_k which appears in the spectral decomposition (7) of ρ has a decomposition $\psi_k = \phi_{k,1} + \phi_{k,2}$ with

$$h\phi_{k,1} = \omega_1 \phi_{k,1}, \;\; h\phi_{k,2} = \omega_2 \phi_{k,2} \;\; \textit{and} \;\; \langle \phi_{k,\varepsilon}, \phi_{l,\eta} \rangle = \frac{1}{2} \delta_{k,l} \delta_{\varepsilon,\eta}$$

for all $k, l \in \{1, \ldots n\}$ *and for all* $\varepsilon, \eta \in \{1, 2\}$.

Proof. As in the case of pure states we start from

$$\frac{\mathrm{d}}{\mathrm{d}t} P_\rho(t) = \frac{\mathrm{d}}{\mathrm{d}t} \left\langle \mathrm{e}^{\mathrm{i}ht} \Pi \mathrm{e}^{-\mathrm{i}ht} \right\rangle_\rho = \mathrm{i} \left\langle \mathrm{e}^{\mathrm{i}ht} [h, \Pi] \, \mathrm{e}^{-\mathrm{i}ht} \right\rangle_\rho = \mathrm{i} \left\langle [h, \Pi] \right\rangle_{\rho_t} .$$

The generalized uncertainty relation for the mixed state ρ_t applied to the pair of observables (h, Π) reads

$$2 (\Delta h)_{\rho_t} (\Delta \Pi)_{\rho_t} \geq \left| \langle [h, \Pi] \rangle_{\rho_t} \right| .$$

From $\Pi^2 = \Pi$ we obtain $(\Delta \Pi)^2_{\rho_t} = P_\rho(t) (1 - P_\rho(t))$ and therefrom the estimate

$$\left| \frac{\mathrm{d}}{\mathrm{d}t} P_\rho(t) \right| \leq 2 (\Delta h)_\rho \sqrt{P_\rho(t) (1 - P_\rho(t))}$$

for all $t \in \mathbb{R}$.

The alternatives (i) and (ii) follow from this for $t > 0$ in exactly the same way as in the case of the pure state survival probability P_ϕ. Since, however, the mixed state survival probability P_ρ need not be an even function, the case $t < 0$ needs a separate consideration: The case $t < 0$ is transformed into the case $t > 0$ by replacing the Hamiltonian h through $-h$. Since the variance of $-h$ in the state ρ is the same as that of h, the alternatives (i) and (ii) hold for for $t < 0$ unchanged.

Suppose now that alternative (ii) holds. Then $P_\rho(t) = \cos^2((\Delta h)_\rho t) = 1 - t^2 (\Delta h)_\rho^2 + \mathrm{O}\left(t^4\right)$ for $t \to 0$. Thus $-P''_\rho(0)/2 = (\Delta h)_\rho^2$ holds. From equation (9) we then obtain

$$(\Delta h)_\rho^2 = \sum_{k=1}^{n} \lambda_k (\Delta h)_{\psi_k}^2 - \sum_{\substack{k,l=1 \\ k \neq l}}^{n} \lambda_l \left|\langle \psi_k, h\psi_l \rangle\right|^2 . \tag{10}$$

Now a general result of probability theory says that the variance of a stochastic variable under a mixture of probability measures is greater or equal to the mixture of individual variances, or more specifically applied to the present context it says that

$$(\Delta h)_\rho^2 - \sum_{k=1}^{n} \lambda_k (\Delta h)_{\psi_k}^2 = \sum_{k=1}^{n} \sum_{l=k+1}^{n} \lambda_k \lambda_l \left(\langle h \rangle_{\psi_k} - \langle h \rangle_{\psi_l} \right)^2 \geq 0. \tag{11}$$

The proof of equation (11) is given in the appendix. From the equations (11), and (10) it thus follows that

$$0 \geq - \sum_{\substack{k,l=1 \\ k \neq l}}^{n} \lambda_l \left|\langle \psi_k, h\psi_l \rangle\right|^2 = \sum_{k=1}^{n} \sum_{l=k+1}^{n} \lambda_k \lambda_l \left(\langle h \rangle_{\psi_k} - \langle h \rangle_{\psi_l} \right)^2 \geq 0.$$

Thus both sides of this equation must vanish and $\langle \psi_k, h\psi_l \rangle = 0$ and $\langle h \rangle_{\psi_k} = \langle h \rangle_{\psi_l}$ follows for all (k,l) with $k \neq l$. Furthermore we have

$$(\Delta h)_\rho^2 = \sum_{k=1}^{n} \lambda_k (\Delta h)_{\psi_k}^2 .$$

From (8) it follows for $P_\rho(t) = \cos^2\left((\Delta h)_\rho t\right) = \frac{1}{2}\left(1 + \cos\left(2 (\Delta h)_\rho t\right)\right)$ that

$$\frac{1}{2}\left(1 + \cos\left(2 (\Delta h)_\rho t\right)\right) = \sum_{k=1}^{n} \lambda_k P_{\psi_k}(t) + \sum_{\substack{k,l=1 \\ k \neq l}}^{n} \lambda_l \left|\left\langle \psi_k, \mathrm{e}^{-\mathrm{i}ht} \psi_l \right\rangle\right|^2 . \tag{12}$$

This implies that each of the even functions P_{ψ_k} is a real linear combination of the constant function 1 and $\cos(2(\Delta h)_\rho t)$. Thus we have for all $t \in \mathbb{R}$

$$\begin{aligned} P_{\psi_k}(t) &= A_k + B_k \cos\left(2 (\Delta h)_\rho t\right) = A_k + B_k - 2B_k \sin^2\left((\Delta h)_\rho t\right) \\ &= 1 - 2B_k \sin^2\left((\Delta h)_\rho t\right). \end{aligned}$$

with constants $A_k, B_k \in \mathbb{R}$ such that $P_{\psi_k}(0) = A_k + B_k = 1$. From $0 \leq P_{\psi_k}(t) \leq 1$ it follows that $0 \leq 2B_k \leq 1$.

Thus P_{ψ_k} obeys for $t \to 0$

$$P_{\psi_k}(t) = 1 - 2B_k (\Delta h)_\rho^2 t^2 + \mathrm{O}\left(t^4\right).$$

Taking into account that $\langle \psi_k, h\psi_l \rangle = 0$ for $k \neq l$ the right hand side of equation (12) obeys

$$\sum_{k=1}^{n} \lambda_k P_{\psi_k}(t) + \sum_{\substack{k,l=1 \\ k\neq l}}^{n} \lambda_l \left|\left\langle \psi_k, \mathrm{e}^{-\mathrm{i}ht}\psi_l \right\rangle\right|^2 = \sum_{k=1}^{n} \lambda_k \left(1 - 2B_k \left(\Delta h\right)_\rho^2 t^2\right) + \mathrm{O}\left(t^4\right).$$

Thus we conclude from equation (12) that

$$1 - \left(\Delta h\right)_\rho^2 t^2 = \sum_{k=1}^{n} \lambda_k \left(1 - 2B_k \left(\Delta h\right)_\rho^2 t^2\right).$$

From this it follows that $\sum_{k=1}^{n} \lambda_k 2B_k = 1$, which in turn implies by means of $0 \leq 2B_k \leq 1$ that $2B_k = 1$ for all k. Thus we have $\left(\Delta h\right)_{\psi_k} = \left(\Delta h\right)_\rho$ and

$$P_{\psi_k}(t) = \cos^2\left(\left(\Delta h\right)_\rho t\right)$$

for each k. From (12) it now follows that

$$\sum_{\substack{k,l=1 \\ k\neq l}}^{n} \lambda_l \left|\left\langle \psi_k, \mathrm{e}^{-\mathrm{i}ht}\psi_l \right\rangle\right|^2 = 0$$

for all t. For each of the vectors ψ_k alternative (ii) of proposition 1 is thus realized. From $\langle h \rangle_{\psi_k} = \langle h \rangle_{\psi_l}$ and from $\left(\Delta h\right)_{\psi_k} = \left(\Delta h\right)_\rho$ it finally follows that the eigenvalues $\omega_{k,\varepsilon}$ in $h\phi_{k,\varepsilon} = \omega_{k,\varepsilon}\phi_{k,\varepsilon}$ do not depend on k.

The inverse statement is obvious by direct computation. ∎

4. Appendix: Differential inequalities

Let I, J be two closed real intervals with $(\xi, \eta) \in I \times J$ and let $f : I \times J \to \mathbb{R}$ be continuous. Then the following results can be found in either Chapt. I, §9, sects. VI and VIII (pp. 73 - 75) of Ref. [11] or in Chapt. II, §8, sects. IX and X (pp. 67 - 69) of Ref. [12].

Proposition 3 *The initial value problem* $y(\xi) = \eta$ *of the differential equation* $y' = f(x, y)$ *has two solutions* y_* *and* y^* *which both extend to the boundary of* $I \times J$ *such that any other solution* y *of this initial value problem obeys* $y_*(x) \leq y(x) \leq y^*(x)$ *wherever both sides of an inequality are defined.*§

Proposition 4 *Let* $v : I \to J$ *and* $w : I \to J$ *be* C^1 *functions with*

$$\begin{aligned} v(\xi) &\leq \eta \text{ and } v'(x) \leq f(x, v(x)) \text{ for all } x \geq \xi \\ w(\xi) &\geq \eta \text{ and } w'(x) \geq f(x, w(x)) \text{ for all } x \geq \xi \end{aligned}$$

then holds $v(x) \leq y^*(x)$ *and* $w(x) \geq y_*(x)$ *for all* $x \geq \xi$ *wherever both sides of an inequality are defined.*

§ The solution y_* is called minimal and y^* is called maximal. Yet it is also common to call any solution of maximal domain a maximal solution. These two notions of maximal solutions thus should not be confused.

5. Appendix: Variance and mixing

Lemma 5 *Let $\rho : \mathcal{H} \to \mathcal{H}$ be a density operator on the finite dimensional Hilbert space $\mathcal{H}$ with its spectral decomposition as given by equation (7). Let $h : \mathcal{H} \to \mathcal{H}$ be linear and symmetric. We abbreviate $\langle h\rangle_{\psi_k}$ by $\langle h\rangle_k$. Then holds*

$$(\Delta h)^2_\rho = \sum_{k=1}^n \lambda_k \left(\Delta h\right)^2_k + \frac{1}{2}\sum_{k,l=1}^n \lambda_k\lambda_l \left(\langle h\rangle_k - \langle h\rangle_l\right)^2 .$$

Proof. First we observe that

$$\begin{aligned}(\Delta h)^2_\rho &= \left\langle h^2\right\rangle_\rho - \langle h\rangle^2_\rho = \sum_{k=1}^n \lambda_k \left\langle h^2\right\rangle_k - \sum_{k,l=1}^n \lambda_k\lambda_l \langle h\rangle_k \langle h\rangle_l \\ &= \sum_{k=1}^n \lambda_k \left(\Delta h\right)^2_k + \sum_{k=1}^n \lambda_k \langle h\rangle^2_k - \sum_{k,l=1}^n \lambda_k\lambda_l \langle h\rangle_k \langle h\rangle_l .\end{aligned}$$

From the last term we extract the contribution with $k = l$ to obtain for $M := (\Delta h)^2_\rho - \sum_{k=1}^n \lambda_k \left(\Delta h\right)^2_k$

$$M = \sum_{k=1}^n \lambda_k \langle h\rangle^2_k - \sum_{k=1}^n \lambda_k^2 \langle h\rangle^2_k - \sum_{k=1}^n \sum_{l=1,l\neq k}^n \lambda_k\lambda_l \langle h\rangle_k \langle h\rangle_l .$$

In the second sum of this we replace $\lambda_k^2 = \lambda_k \left(1 - \sum_{l\neq k} \lambda_l\right)$ which yields

$$\begin{aligned}M &= \sum_{k=1}^n \sum_{l=1,l\neq k}^n \lambda_k\lambda_l \langle h\rangle^2_k - \sum_{k=1}^n \sum_{l=1,l\neq k}^n \lambda_k\lambda_l \langle h\rangle_k \langle h\rangle_l \\ &= \sum_{k=1}^n \sum_{l=1,l\neq k}^n \lambda_k\lambda_l \left(\langle h\rangle^2_k - \langle h\rangle_k \langle h\rangle_l\right) \\ &= \frac{1}{2}\sum_{k=1}^n \sum_{l=1,l\neq k}^n \lambda_k\lambda_l \left(\langle h\rangle^2_k + \langle h\rangle^2_l - 2\langle h\rangle_k \langle h\rangle_l\right) \\ &= \frac{1}{2}\sum_{k=1}^n \sum_{l=1,l\neq k}^n \lambda_k\lambda_l \left(\langle h\rangle_k - \langle h\rangle_l\right)^2 .\end{aligned}$$

■

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